

Chapter 6

Matrix elements

6.1 Matrix elements of spherical harmonics

The spherical harmonics $Y_{lm}(\theta\varphi)$ were defined by Eq. (1.25) in terms of associated Legendre polynomials, $P_l^m(\cos\theta)$ of the first kind,

$$\left. \begin{aligned} Y_{lm}(\theta\varphi) &= (-1)^m \left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right)^{1/2} P_l^m(\cos\theta) \exp(im\varphi) \\ P_l^m(\cos\theta) &= (\sin\theta)^m \frac{d^m}{d(\cos\theta)^m} P_l(\cos\theta) \end{aligned} \right\} \quad (6.1)$$

$P_l(\cos\theta)$ are the Legendre polynomials. The spherical harmonics satisfy the following relations

$$\left. \begin{aligned} Y_{l-m}(\theta\varphi) &= (-1)^m Y_{lm}^*(\theta\varphi) \\ Y_{lm}(\pi - \theta\varphi + \pi) &= (-1)^l Y_{lm}(\theta\varphi) \end{aligned} \right\} \quad (6.2)$$

It is often more convenient to work with $C_m^l(\theta\varphi)$ which are defined by the relation

$$C_m^l(\theta\varphi) = \sqrt{\frac{4\pi}{2l+1}} Y_{lm}(\theta\varphi) \quad (6.3)$$

We now turn our attention to matrix elements of the type

$$\langle l'm' | Y_{kq} | lm \rangle = \int d\theta d\varphi \sin\theta Y_{l'm'} Y_{kq} Y_{lm} \quad (6.4)$$

Integrals such as Eq. (6.4) are called Gaunt's coefficients and do often appear in atomic physics, *c.f.* crystal field splitting in $l^{(N)}$ systems (note that we work within the Y_{lm} basis). Wigner-Eckart theorem applied to Eq. (6.4) give for the Gaunt's coefficients

$$\langle l'm' | Y_{kq} | lm \rangle = (-1)^{l'-m'} \begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} \langle l' || Y_k || l \rangle \quad (6.5)$$

It should once again be stressed that thanks to the Wigner-Eckart theorem, the geometrical dependencies in Eq. (6.5) can be factored out and are controlled by the

3j-symbol. This indeed simplifies the computation of more difficult matrix elements. To evaluate the reduced matrix element of Eq. (6.5) we note that

$$Y_{kq}|lm\rangle = \sum_{l'm'} |l'm'\rangle \langle l'm'|Y_{kq}|lm\rangle \quad (6.6)$$

where we just have multiplied the right hand side with a “1”. Eq. (6.5) into Eq. (6.6) and multiplying both sides with

$$\sum_{qm} \begin{pmatrix} l'' & k & l \\ -m' & q & m \end{pmatrix}$$

give us a nice looking expression

$$\begin{aligned} \sum_{qm} \begin{pmatrix} l'' & k & l \\ -m' & q & m \end{pmatrix} Y_{kq}|lm\rangle = \\ \sum_{l'm'qm} |l'm'\rangle \begin{pmatrix} l'' & k & l \\ -m' & q & m \end{pmatrix} \begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} (-1)^{l'-m'} \langle l' || Y_k || l \rangle \end{aligned} \quad (6.7)$$

By using Eq. (2.20), Eq. (6.7) simplifies to

$$\sum_{qm} \begin{pmatrix} l'' & k & l \\ -m' & q & m \end{pmatrix} Y_{kq}|lm\rangle = |l'm'\rangle (-1)^{l''-m'} / [l''] \langle l'' || Y_k || l \rangle \quad (6.8)$$

Multiply from the left with $\langle \hat{n} |$ (note that $\langle \hat{n} | lm \rangle = Y_{lm}(\hat{n})$). The new expression is true for any $\theta\varphi$, *e.g.* $\theta = 0$ which gives using $Y_{lm}(0\varphi) = \sqrt{[l]/(4\pi)}\delta_{m0}$ and the fact that $m' = q + m$ (Eq. (2.23))

$$\langle l' || Y_k || l \rangle = (-1)^{l'} \sqrt{[l'] [k] [l] / (4\pi)} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \quad (6.9)$$

Note that we changed the variable name $l'' \rightarrow l'$. The Gaunt's coefficient now become

$$\langle l'm' | Y_{kq} | lm \rangle = (-1)^{m'} \sqrt{[l'] [k] [l] / (4\pi)} \begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \quad (6.10)$$

which is our final result. Eq. (6.2) together with Eq. (6.10) give the following nice expression for the seemingly difficult integral

$$\int Y_{l_1 m_1} Y_{l_2 m_2} Y_{l_3 m_3} \sin \theta d\theta d\varphi = \sqrt{[l_1] [l_2] [l_3] / (4\pi)} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad (6.11)$$

The reason for the definition of C_q^k in Eq. (6.3) becomes obvious through Eqs. (6.9) and (6.10) because

$$\langle l'm' | C_q^k | lm \rangle = (-1)^{m'} \sqrt{[l'] [l]} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} \quad (6.12)$$

and

$$\langle l' || C^k || l \rangle = (-1)^{l'} \sqrt{[l'] [l]} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \quad (6.13)$$

There exist efficient algorithms for the calculation of nj -symbols, and therefore integrals such as those above can be handled very nicely.

6.2 Matrix elements of tensorproducts

In Eq. (4.21) we defined the product of two tensor operators, $X_Q^{(K)} = (T_{q_1}^{(k_1)} U_{q_2}^{(k_2)})_Q^{(K)}$, and proved it transformed according to Eq. (4.16) under a rotation. We now shall investigate the matrix element of a tensor product. Applying the Wigner-Eckart theorem and using the definition of a tensor product Eq. (4.21) we see

$$\begin{aligned}
\langle \gamma' J' M' | X_Q^{(K)} | \gamma J M \rangle &= \\
\sum_{q_1 q_2 \gamma'' J'' M''} \langle \gamma' J' M' | T_{q_1}^{(k_1)} | \gamma'' J'' M'' \rangle \langle \gamma'' J'' M'' | U_{q_2}^{(k_2)} | \gamma J M \rangle \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle &= \\
\sum_{q_1 q_2 \gamma'' J'' M''} (-1)^{J' - M' + J'' - M'' + k_1 - k_2 + Q} \sqrt{[K]} \times \\
\begin{pmatrix} J' & k_1 & J'' \\ -M' & q_1 & M'' \end{pmatrix} \begin{pmatrix} J'' & k_2 & J \\ -M'' & q_2 & M \end{pmatrix} \begin{pmatrix} k_1 & k_2 & K \\ q_1 & q_2 & -Q \end{pmatrix} \times \\
\langle \gamma' J' | T^{(k_1)} | \gamma'' J'' \rangle \langle \gamma'' J'' | U^{(k_2)} | \gamma J \rangle & \quad (6.14)
\end{aligned}$$

where we “as usual” have inserted the “1”. Wigner-Eckart theorem on the left hand side of Eq. (6.14) gives

$$\langle \gamma' J' M' | X_Q^{(K)} | \gamma J M \rangle = (-1)^{J' - M'} \begin{pmatrix} J' & K & J \\ -M' & Q & M \end{pmatrix} \langle \gamma' J' | X^{(K)} | \gamma J \rangle \quad (6.15)$$

The obvious problem to solve is to get an expression for the reduced matrix element on the right hand side of Eq. (6.15). Multiply Eq. (6.15) with

$$\sum_{M M' Q} \begin{pmatrix} J' & K & J \\ -M' & Q & M \end{pmatrix} \quad (6.16)$$

and use the relation Eq. (2.20), *c.f.* Eqs. (6.7) and (6.8), we arrive at

$$\begin{aligned}
\langle \gamma' J' | X^{(K)} | \gamma J \rangle &= \sum_{q_1 q_2 Q M M' \gamma'' J''} (-1)^{J'' - M'' + k_1 - k_2 + Q} \sqrt{[K]} \begin{pmatrix} J' & K & J \\ -M' & Q & M \end{pmatrix} \\
&\times \begin{pmatrix} J' & k_1 & J'' \\ -M' & q_1 & M'' \end{pmatrix} \begin{pmatrix} J'' & k_2 & J \\ -M'' & q_2 & M \end{pmatrix} \begin{pmatrix} k_1 & k_2 & K \\ q_1 & q_2 & -Q \end{pmatrix} \\
&\times \langle \gamma' J' | T^{(k_1)} | \gamma'' J'' \rangle \langle \gamma'' J'' | U^{(k_2)} | \gamma J \rangle \quad (6.17)
\end{aligned}$$

Massaging Eq. (6.17) and the definition of 6j-symbols in term of 3j-symbols, Eq. (2.42), finally give us

$$\begin{aligned}
\langle \gamma' J' | X^{(K)} | \gamma J \rangle &= \sqrt{[K]} \sum_{\gamma'' J''} (-1)^{J + J' + K} \left\{ \begin{matrix} k_1 & k_2 & K \\ J & J' & J'' \end{matrix} \right\} \times \\
&\langle \gamma' J' | T^{(k_1)} | \gamma'' J'' \rangle \langle \gamma'' J'' | U^{(k_2)} | \gamma J \rangle \quad (6.18)
\end{aligned}$$

The above expression is valid whether $T^{(k_1)}$ and $U^{(k_2)}$ act on the same system or not. It often occurs that the two tensor operators act on different systems, *c.f.* the electrostatic interaction between two electrons where $1/r_{12} \propto C_1^{(k)} \cdot C_2^{(k)}$, or the spin-orbit

interaction $s \cdot l$. We therefore want to express Eq. (6.18) in terms of the reduced matrix elements for the decoupled systems $\langle \gamma' j'_1 || T^{(k_1)} || \gamma'' j_1 \rangle$ and $\langle \gamma'' j'_2 || U^{(k_2)} || \gamma j_2 \rangle$ if $U^{(k_2)}$ act on the 2-system and $T^{(k_1)}$ on the 1-system. We start with $\langle \gamma j'_1 j'_2 J' M' | X_Q^{(K)} | \gamma j_1 j_2 J M \rangle$ and change representation to $m_1 m_2$ and $m'_1 m'_2$ plus use Eq. (4.21) (definition of the two tensor operator product)

$$\begin{aligned} \langle \gamma j'_1 j'_2 J' M' | X_Q^{(K)} | \gamma j_1 j_2 J M \rangle &= \sum_{m'_1 m'_2 m_1 m_2 q_1 q_2} \langle j'_1 j'_2 J' M' | j'_1 j'_2 m'_1 m'_2 \rangle \times \\ &\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M \rangle \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle \times \\ &\langle \gamma j'_1 j'_2 m'_1 m'_2 | T_{q_1}^{(k_1)} U_{q_2}^{(k_2)} | \gamma j_1 j_2 m_1 m_2 \rangle \end{aligned} \quad (6.19)$$

Using

$$\sum_{\gamma'' j''_1 j''_2 m''_1 m''_2} |\gamma'' j''_1 j''_2 m''_1 m''_2 \rangle \langle \gamma'' j''_1 j''_2 m''_1 m''_2| = 1$$

and the definition of $3j$ -symbols Eq. (2.16), Eq. (6.19) then takes the form (the sum is over $m'_1 m'_2 m_1 m_2 q_1 q_2 \gamma'' j''_1 j''_2 m''_1 m''_2$)

$$\begin{aligned} \langle \gamma j'_1 j'_2 J' M' | X_Q^{(K)} | \gamma j_1 j_2 J M \rangle &= \sum (-1)^{j'_1 - j'_2 + M' + j_1 - j_2 + M + k_1 - k_2 + Q} \sqrt{[J'] [J] [K]} \times \\ &\begin{pmatrix} j'_1 & j'_2 & J' \\ m'_1 & m'_2 & -M' \end{pmatrix} \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix} \begin{pmatrix} k_1 & k_2 & K \\ q_1 & q_2 & -Q \end{pmatrix} \times \\ &\langle \gamma' j'_1 j'_2 m'_1 m'_2 | T_{q_1}^{(k_1)} | \gamma'' j''_1 j''_2 m''_1 m''_2 \rangle \langle \gamma'' j''_1 j''_2 m''_1 m''_2 | U_{q_2}^{(k_2)} | \gamma j_1 j_2 m_1 m_2 \rangle \end{aligned} \quad (6.20)$$

Up to now we have not assumed anything concerning which system the tensor operator acts on. If for example $T_{q_1}^{(k_1)}$ acts on the 1-system and $U_{q_2}^{(k_2)}$ act on the 2-system, the matrix elements on the right hand side of Eq. (6.20) reduce to

$$\left. \begin{aligned} &\langle \gamma' j'_1 m'_1 | T_{q_1}^{(k_1)} | \gamma'' j''_1 m''_1 \rangle \delta_{j'_2 j''_2} \delta_{m'_2 m''_2} \\ &\langle \gamma'' j''_2 m''_2 | U_{q_2}^{(k_2)} | \gamma j_2 m_2 \rangle \delta_{j'_1 j_1} \delta_{m'_1 m_1} \end{aligned} \right\} \quad (6.21)$$

Wigner-Eckart on both sides of Eq. (6.20) and using the assumption Eq. (6.21) we get for the reduced matrix element $\langle \gamma' j'_1 j'_2 J' || X^{(K)} || \gamma j_1 j_2 J \rangle$ after having multiplied by

$$\sum_{MM'Q} \begin{pmatrix} J' & K & J \\ -M' & Q & M \end{pmatrix},$$

and used the orthogonality relation for $3j$ -symbols, *c.f.* Eqs. (6.15) and (6.17), and the definition of $9j$ -symbols in terms of $3j$ -symbols Eq. (2.69),

$$\begin{aligned} \langle \gamma' j'_1 j'_2 J' || X^{(K)} || \gamma j_1 j_2 J \rangle &= \\ \sqrt{[J] [J'] [K]} \left\{ \begin{array}{ccc} j'_1 & j_1 & k_1 \\ j'_2 & j_2 & k_2 \\ J' & J & K \end{array} \right\} \sum_{\gamma''} \langle \gamma' j'_1 || T^{(k_1)} || \gamma'' j_1 \rangle \langle \gamma'' j'_2 || U^{(k_2)} || \gamma j_2 \rangle \end{aligned} \quad (6.22)$$

remembering

$$\begin{aligned} & \langle \gamma' j'_1 j'_2 J' M' | X_Q^{(K)} | \gamma j_1 j_2 J M \rangle = \\ & (-1)^{J'-M'} \begin{pmatrix} J' & K & J \\ -M' & Q & M \end{pmatrix} \langle \gamma' j'_1 j'_2 J' || X^{(K)} || \gamma j_1 j_2 J \rangle \end{aligned} \quad (6.23)$$

From Eq. (2.71) we know that a $9j$ -symbol reduce essentially to a $6j$ -symbol when one of its arguments is zero. Thus, Eq. (6.23) for a scalar product (S) becomes, *c.f.* Eqs. (4.23) and (4.24), using Eq. (4.21),

$$S = (T^{(k)} \cdot U^{(k)}) = \sum_q (-1)^q T_q^{(k)} U_{-q}^{(k)} = (-1)^k \sqrt{[k]} X_0^{(0)} \quad (6.24)$$

$$\begin{aligned} & \langle \gamma' j'_1 j'_2 J' M' | S | \gamma j_1 j_2 J M \rangle = \\ & (-1)^{J'-M'} \begin{pmatrix} J' & 0 & J \\ -M' & 0 & M \end{pmatrix} \langle \gamma' j'_1 j'_2 J' || S || \gamma j_1 j_2 J \rangle = \\ & \delta_{M'M} \delta_{J'J} ([J])^{-1/2} (-1)^k \sqrt{[k]} \sqrt{[J][J']} \left\{ \begin{matrix} j'_1 & j_1 & k \\ j'_2 & j_2 & k \\ J' & J & 0 \end{matrix} \right\} \times \\ & \sum_{\gamma''} \langle \gamma' j'_1 || T^{(k)} || \gamma'' j_1 \rangle \langle \gamma'' j'_2 || U^{(k)} || \gamma j_2 \rangle = \\ & \delta_{M'M} \delta_{J'J} (-1)^{j_1+j_2+J} \left\{ \begin{matrix} j'_1 & j_1 & k \\ j_2 & j'_2 & J \end{matrix} \right\} \sum_{\gamma''} \langle \gamma' j'_1 || T^{(k)} || \gamma'' j_1 \rangle \langle \gamma'' j'_2 || U^{(k)} || \gamma j_2 \rangle \end{aligned} \quad (6.25)$$

This result corresponds to Eq. (38) in Racah's classic paper II [3]. Racah continued to massage matrix elements of the types discussed so far, and we will do the same.

We first recall that an odd permutation of rows/columns change sign on the $9j$ -symbol if $\sum_i J_i = \text{odd}$. Therefore

$$\left\{ \begin{matrix} j'_1 & j_1 & k \\ j_2 & j_2 & 0 \\ J' & J & k \end{matrix} \right\} = (-1)^{j'_1+j_2+J+k} ([k][j_2])^{-1/2} \left\{ \begin{matrix} j'_1 & j_1 & k \\ J & J' & j_2 \end{matrix} \right\} \quad (6.26)$$

Next note that

$$\langle \gamma j'_2 || 1 || \gamma j_2 \rangle = \delta_{j'_2 j_2} (-1)^{j_2-m_2} / \begin{pmatrix} j_2 & 0 & j_2 \\ -m_2 & 0 & m_2 \end{pmatrix} = \sqrt{[j_2]} \quad (6.27)$$

according to Eq. (2.70). Eq. (6.22) now give using Eqs. (6.26), (6.27), $k_2 = 0$ and $U_2^{(k)} = 1$ (U acting on system 2)

$$\begin{aligned} & \langle \gamma' j'_1 j'_2 J' || T^{(k)} || \gamma j_1 j_2 J \rangle = \\ & \delta_{j'_2 j_2} (-1)^{j'_1+j_2+J+k} \sqrt{[J][J']} \left\{ \begin{matrix} j'_1 & j_1 & k \\ J & J' & j_2 \end{matrix} \right\} \langle \gamma' j'_1 || T^{(k)} || \gamma j_1 \rangle \end{aligned} \quad (6.28)$$

and for $k_1 = 0$ and $T_1^{(k)} = 1$

$$\begin{aligned} \langle \gamma' j'_1 j'_2 J' || U^{(k)} || \gamma j_1 j_2 J \rangle = \\ \delta_{j'_1 j_1} (-1)^{j_1 + j'_2 + J' + k} \sqrt{[J][J']} \left\{ \begin{matrix} j'_2 & j_2 & k \\ J & J' & j_1 \end{matrix} \right\} \langle \gamma' j'_2 || U^{(k)} || \gamma j_2 \rangle \end{aligned} \quad (6.29)$$

The last two equations correspond to Racahs Eqs. (44a) and (44b) in II. The usefulness of these types of matrix elements become obvious when working on “real” problems.